1,3-Dichlorobenzene

541-73-	DTXSID602205

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 175 °C

Global applicability domain: Inside

Local applicability domain index: 6.97e-01

Confidence level: 8.12e-01

Nearest Neighbors from the Training Set

Image not found

Bromobenzene Measured: 156 Predicted: 175 Image not found

1,3-Dichlorobenzene Measured: 173 Predicted: 175 Image not found

Benzene, (methylthio)-Measured: 193 Predicted: 191

Image not found

1,2-Dichlorobenzene Measured: 180 Predicted: 174 Image not found

1,4-Dichlorobenzene Measured: 174 Predicted: 175